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ABSTRACT

The publication describes a convenient form of one-dimensional equations describing the multi-phase flows associated with the initiation of novel warheads. The model, which has been proposed earlier for the case of two phases, is extended to the case of multi-phase flows. The generalized pressure and energy, which are used in the theory of mixtures, are linked through a thermodynamic potential within the present formulation.

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Executive Summary

Recent conflicts and peacekeeping missions have revealed the need for novel warheads able to selectively release the blast and fragmentation energy against prescribed targets to minimise collateral damage. Analysis of these new warheads is impossible without consideration of multi-phase flows involved in the warhead detonation. Warhead components, can include composite and inhomogeneous explosives, and fragmentation warheads include fragment particles, which could be treated as an additional phase of the warhead flow. It also provides the potential capability of tailoring the blast and impact energy release at a given time and location that would be of significant benefit to the optimisation of the warhead effects against specified targets.

Numerical analysis of the warhead effects involves at least two stages:

i) construction of kinetic relationships, which are responsible for the internal and chemical processes in the products involved in the multi-phase flow. The fitting of these relationships to available test data also involves their verification with calculations, employing an accurate numerical scheme; and

ii) a hydrocode/CFD study of the target effects with a multi-dimensional code (likely to be a commercial code with the possibility of incorporation of the model), which employs the multi-phase model with the closing kinetic relations verified during the previous stage.

The verification process is likely to be conducted with a one-dimensional code because the space accuracy needed for the verification is hard to achieve in the multi-dimensional case due to resource limitations. For analysis of the processes involved in the warhead detonation we need a numerical method, which would describe accurately elementary processes (shock and rarefaction) composing the whole picture of expansion of the detonation products and their interaction with the target. The only scheme, which explicitly involves solutions adjusted to the elementary problems (Riemann problems) is the Godunov method along with the family of follow-up schemes (TVD, B. van-Leer scheme, etc). To apply this scheme to the equations of the model, certain requirements are necessary for the model's system to be satisfied: the equations should be written out in the form of conservation laws and elementary solutions should be designed when building up an appropriate Riemann solver.

Unfortunately, among many models, having been developed recently, only a few can be formulated in the form of conservation laws. Very significant progress in this direction has been made by E. Romensky, who proposed the conservation law formulations for a large

variety of models, including a two-phase model from which the present consideration starts.

The present report considers the modelling of two-phase flows and suggests a new formulation of the model resulting in a thermodynamic identity that is applicable to the case of one-dimensional flows. This formulation establishes a clear link between the pressure and energy definitions, embracing the diffusive constituents, which are widely used in the theory of mixtures [3], through this thermodynamic identity. The present formulation is more convenient for construction of a Riemann solver and its use in the Godunov scheme. This formulation is extendable to the case of multiple phases with complete thermodynamic closure of the model, using only thermodynamic potential.

Results of the present study are important for construction of the algorithms and numerical methods, which are necessary for the verification of kinetic equations involved in the process of detonation of advanced warheads. Extension of the model to the case of multiple phases is critical for analysis of real-life warheads, because novel volumetric and fragmentation warheads involve, as a rule, more than two phases in actual engagement scenarios.

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Anatoly Resnyansky obtained a MSc in Applied Mathematics and Mechanics from the Novosibirsk State University (Russia) in 1979. In 1979-1995 he worked in the Lavrentyev Institute of Hydrodynamics (Russian Academy of Science) in the area of constitutive modelling for problems of high-velocity impact. Anatoly obtained a PhD in Physics and Mathematics from the Institute of Hydrodynamics in 1985. In 1996-1998 he worked in private industry in Australia. He joined the Terminal Effects group of the Weapons Systems Division (DSTO) in 1998 where his current research interests include constitutive modelling and material characterisation at the high strain rates, ballistic testing and simulation, and theoretical and experimental analysis of the warhead effects.

Contents

1. Introduction

Many modern warheads employ single- or multi-stage initiation designs involving several energetic and filling constituents. Thus, chemical and mechanical inhomogeneities are widely used for arranging a tailored energy release such as delayed reaction/initiation, afterburn, etc. Such the complex energetic materials involve multiple reactive components and require description with models, which are capable of calculating multi-phase flows. Interest in multi-phase flows is spread world-wide due to application of CFD modelling to processes of combustion, heterogeneous detonation, and to processes in gas-liquid and bubble-liquid mixtures. To simulate such the processes, models, comprising of the conservation laws for mass, momentum and energy, associated with each of the phases, are extremely popular; the conservation laws are formulated for partial characteristics (additive characteristics with respect to the common volume, containing several phases) and interconnected by the exchange terms. However, this approach is not very convenient because it involves description of every phase that multiplies the number of equations by the factor equal to the number of phases. On the other side, incorporation of such models in a hydrocode is hard because the majority of commercial hydrocodes operate with a single system of conservation laws complemented with so-called constitutive equations (in the CFD/engineering chemistry communities they are usually called kinetic equations). Many attempts to consider multi-phase medium as an averaged one have been made, including a classic monograph by Truesdell [3]. However, a closed thermodynamic formulation, resulting in an efficient practical realisation, has not been proposed at that time. A variety of models have been recently developed in several papers [4, 5]. However, they are not in the form of conservation laws, that complicates analysis of their thermodynamical correctness and makes application of the Godunov scheme difficult.

The present work employs a consistent approach, enabling us to derive equations in the form of conservation laws; one of the first realizations of this approach has been published in [6]. It invokes the mass averaging over two phases, so the effective averaging parameter involved is the mass fraction of one of the two phases. Realization of this approach as a computer code [6] resulted in significant numerical difficulties associated with the phase exchange (convection) in the areas of high gradients between the phases. A note by Drumheller [7] was important for understanding that one more parameter associated with the phase concentration should be involved in the processes, which accompany phase exchange, reaction processes between the phases, etc. This resulted in introduction of both mass and volumetric concentrations in the averaging process and, as a result, several successful models [2, 8] based on this approach have appeared: the model [2] is an extension of the model [6] for the case of two-phase media with the velocity nonequilibrium (drag) between the phases and [8] is a single-velocity two-phase model with the temperature nonequilibrium resulting in a complete thermodynamic identity, enabling one to formulate the Gibbs potential in its classical form. Formulation [2] provides a thermodynamically correct model, but known solutions of the Riemann problem cannot be easy applied because the pressure and energy characteristics involved in the jump conditions are not deduced from a single potential. The generalized pressure

and energy can be introduced [3], which involve the diffusion fluxes; however, these force-energy characteristics have not been linked within the formulation [2].

The present publication is an enhanced formulation of the model [2] for the one-dimensional case, allowing us to formulate a complete thermodynamic identity, jump conditions in a convenient form for application to the Riemann problem, and to generalize the model for the case of multiple phases, linking directly the presentation [3] for energy and pressure with involvement of diffusive components. The multi-phase generalization is particularly important for many applications because a typical warhead, for instance, of volumetric action may involve at least three phases: gaseous, dispersed, and liquid products.

2. Model of two-phase flows

Let us denote the average density of a two-phase medium by $\rho=m/V$, here m is mass of a representative volume and V is the volume quantity. Similarly, we can define specific densities of the phases $\rho_1=m_1/V_1$ and $\rho_2=m_2/V_2$. Multi-phase theories usually deal with so-called partial densities, which relate the phase masses to the whole volume such as: $\rho'_1=m_1/V$ and $\rho'_2=m_2/V$. The partial characteristics are important because the conservation laws for each phase can actually be formulated only for these characteristics. For the case of media with phases, which are capable of an exchange with mass and momentum, the conservation laws in one-dimensional case take the following form for the first phase:

$$\begin{aligned}
&\frac{\partial \rho_1'}{\partial t}+\frac{\partial \rho_1' u_1}{\partial x}=m_0^*, \\
&\frac{\partial \rho_1' u_1}{\partial t}+\frac{\partial\left(\rho_1' u_1^2+p_1'\right)}{\partial x}=n_0^*, \\
&\frac{\partial \rho_1'\left(e_1+u_1^2/2\right)}{\partial t}+\frac{\partial\left[\rho_1' u_1\left(e_1+u_1^2/2\right)+p_1' u_1\right]}{\partial x}=0,
\end{aligned} \tag{1}$$

and for the second phase:

$$\begin{aligned}
&\frac{\partial \rho_2'}{\partial t}+\frac{\partial \rho_2' u_2}{\partial x}=-m_0^*, \\
&\frac{\partial \rho_2' u_2}{\partial t}+\frac{\partial\left(\rho_2' u_2^2+p_2'\right)}{\partial x}=-n_0^*, \\
&\frac{\partial \rho_2'\left(e_2+u_2^2/2\right)}{\partial t}+\frac{\partial\left[\rho_2' u_2\left(e_2+u_2^2/2\right)+p_2' u_2\right]}{\partial x}=0.
\end{aligned} \tag{2}$$

Here m^*_0 is the mass exchange rate, n^*_0 is the momentum exchange rate, u_i (i=1,2) are velocities of the phases, p'_1 and p'_2 are partial pressures within the phases, e_1 and e_2 are

specific internal energies. Let us denote T – temperature and S – specific entropy, then the thermodynamic identity

$$T\,\mathrm{d}S = \mathrm{d}e + p\,\mathrm{d}V = \mathrm{d}e - p\,\mathrm{d}\rho/\rho^{2}, \tag{3}$$

being applied to each of the phases, enables us to calculate partial pressure and temperature:

$$\begin{aligned} p_1' &= (\rho_1')^2 \, {\partial e_1}/{\partial \rho_1'}, \quad T_1 = {\partial e_1}/{\partial S_1}, \\ p_2' &= (\rho_2')^2 \, {\partial e_2}/{\partial \rho_2'}, \quad T_2 = {\partial e_2}/{\partial S_2}, \end{aligned} \tag{4}$$

if a dependence of specific energy on ρ' and S is given:

$$e_1 = e_1(\rho'_1, S_1)\ , \quad e_2 = e_2(\rho'_2, S_2)\ . \tag{5}$$

It should be noted that definition of the partial pressure is based on the application of the thermodynamic identity with respect to the partial density. Thus, the traditional approach to calculation of two-phase flows is to calculate the systems (1) and (2), pre-selecting the exchange terms m^*_0 and n^*_0, and tabulating the 'equations of state' in the form (5) (for the sake of convenience, we call the relations like (5) as equations of state), using (4) for calculation of pressure and temperature.

The procedure of averaging, having been employed in [6], involves introduction of averaged density, pressure, and velocity. On the present stage we do not individualize the thermal characteristics of the phases; an example how it could be done for a single-velocity material was shown in [8]; therefore, we consider specific entropy to be common for the both phases. We introduce [1, 2, 8] the mass concentration of the first phase as $c = c_1 = m_1/m$, then for the second phase $c_2 = m_2/m = 1 - c$. We can also determine the partial densities, because

$$\rho'_1 = m_1/V = (m_1/m)\cdot(m/V) = \rho c\ , \qquad \rho'_2 = \rho(1-c)\ . \tag{6}$$

Specific energy is an extensive variable, therefore, for a volume containing both phases the average specific energy is

$$e = c\, e_1 + (1-c)\, e_2\,. \tag{7}$$

Introducing volumetric concentration of the first phase as $\theta_1 = \theta = V_1/V$, we can recalculate the specific densities of the phases

$$\rho_1 = m_1/V_1 = (m_1/m)\cdot(m/V)\cdot(V/V_1) = \rho c/\theta\ , \qquad \rho_2 = \rho(1-c)/(1-\theta)\,. \tag{8}$$

Using (7) and (8), we can build up the equation of state for the averaged state, employing the 'local' equations of state $e_1 = e_1(\rho_1, S)$ and $e_2 = e_2(\rho_2, S)$:

$$e(\rho, c, \theta, S) = c\, e_1(\rho c/\theta, S) + (1 - c)\, e_2(\rho(1 - c)/(1 - \theta), S) \ . \tag{9}$$

Averaged velocity u is introduced as

$$u = c\, u_1 + (1 - c)\, u_2 \,, \tag{10}$$

and the velocity difference between the phases, which is proportional to the so-called diffusion velocity [3], was introduced [2, 6] in the form

$$w = u_1 - u_2 \,. \tag{11}$$

Relations (10) and (11) allow us to calculate local velocities via the averaged velocity and the velocity difference:

$$u_1 = u + (1 - c)\, w \quad , \qquad u_2 = u - c\, w \quad . \tag{12}$$

From (6) and (10): $\rho'_1 + \rho'_2 = \rho$ and $\rho'_1 u_1 + \rho'_2 u_2 = \rho\, u$; using these relations and summing up the continuity equations in (1)-(2), we can obtain the continuity equation for the averaged variables:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0\,. \tag{13}$$

Rewriting the continuity equation of (1) with the use of (6) and (11), we can obtain the kinetic equation for the mass concentration:

$$\frac{\partial \rho c}{\partial t} + \frac{\partial [\rho u c + \rho c(1-c)w]}{\partial x} = m_0^* \,. \tag{14}$$

Kinetic equation for the volume concentration is chosen in usual form of conservation within the liquid volume [1, 2, 6]:

$$\frac{\partial \rho \theta}{\partial t} + \frac{\partial \rho u \theta}{\partial x} = \Phi\,, \tag{15}$$

here Φ is a function responsible for the process of phase compaction.

For further derivations we have to calculate pressure in the averaged medium. Firstly, we link the local pressures and densities with the partial ones. In addition to (6), another calculation of the partial density for the first phase gives

$$\rho'_1 = m_1/V = (m_1/V_1)\cdot(V_1/V) = \rho_1\theta \quad , \qquad \rho'_2 = \rho_2(1-\theta) \quad . \tag{16}$$

We consider an alternative to (5) presentation of the equations of state in the form $e_1 = e_1(\rho_1, S)$, $e_2 = e_2(\rho_2, S)$. Then, from (4) and (16) it follows

$$\begin{aligned} p'_1 &= (\rho'_1)^2 \, \partial e_1 / \partial \rho'_1 = (\rho_1\theta)^2 \left[\left(1/\theta\right) \cdot \left(\partial e_1 / \partial \rho_1 \right) \right] = \theta \cdot \rho_1^2 \, \partial e_1 / \partial \rho_1 = \theta \cdot p_1 \quad , \\ p'_2 &= (1-\theta) p_2 \ , \end{aligned} \tag{17}$$

where the following denotations for the local pressures are used:

$$p_1 = \rho_1^2 \, \partial e_1 / \partial \rho_1 \quad , \quad p_2 = \rho_2^2 \, \partial e_2 / \partial \rho_2 \ , \tag{18}$$

with the equations of state given in the form:

$$e_1 = e_1(\rho_1, S) \quad , \qquad e_2 = e_2(\rho_2, S) \ . \tag{19}$$

The momentum conservation laws (second equations of the systems (1) and (2)) give the following momentum equation for the two-phase medium:

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \left[\rho u^2 + p + \rho c(1-c) w^2 \right]}{\partial x} = 0 \ . \tag{20}$$

Here the following relations have been used

$$\begin{aligned} &\rho'_1 u_1 + \rho'_2 u_2 = \rho u \ , \\ &\rho'_1 (u_1)^2 + \rho'_2 (u_2)^2 = \rho u^2 + \rho \, c(1-c) w^2 \ , \end{aligned} \tag{21}$$

and

$$p = p'_1 + p'_2 \ .$$

The latter can also be obtained by direct differentiating of (7) over ρ and gives the relation

$$p = \theta \, p_1 + (1-\theta) \, p_2 \ .$$

The momentum conservation laws of (1-2) can also be rewritten in the following form

$$\frac{\partial u_1}{\partial t} + u_1 \frac{\partial u_1}{\partial x} + \frac{1}{\rho_1'} \frac{\partial p_1'}{\partial x} = \left(n_0^* - m_0^* u_1\right) / \rho_1' ,$$

$$\frac{\partial u_2}{\partial t} + u_2 \frac{\partial u_2}{\partial x} + \frac{1}{\rho_2'} \frac{\partial p_2'}{\partial x} = -\left(n_0^* - m_0^* u_2\right) / \rho_2' .$$

When using the relation

$$(u_1)^2 - (u_2)^2 = 2uw + (1 - 2c)w^2 , \tag{22}$$

we can derive the equation for the velocity difference:

$$\frac{\partial w}{\partial t} + \frac{\partial \left[uw + (1-2c) w^2 / 2\right]}{\partial x} + \frac{1}{\rho_1'} \frac{\partial p_1'}{\partial x} - \frac{1}{\rho_2'} \frac{\partial p_2'}{\partial x} = \Psi ,$$

where

$$\Psi = \frac{\left\{n_0^* - m_0^* \left[u + (1-c) w\right]\right\}}{\rho c} + \frac{\left\{n_0^* - m_0^* \left[u - cw\right]\right\}}{\rho (1-c)} .$$

To simplify the equation, a chemical potential n is introduced [2], which could be equal to the classical Gibbs potential if the energy exchange is properly introduced [8]. The potential is defined as follows

$$n = e_c = e_1 - e_2 + p_1 / \rho_1 - p_2 / \rho_2 .$$

Noting that $p_i / \rho_i = p'_i / \rho'_i$, we can simplify the last kinetic equation as follows:

$$\frac{\partial w}{\partial t} + \frac{\partial \left[uw + (1-2c) w^2 / 2 + n\right]}{\partial x} = \Psi . \tag{23}$$

The last set of conservation laws in (1)-(2) deals with the energy conservation. To derive it for the averaged medium, we first obtain an auxiliary relation:

$$c(u_1)^2 + (1 - c)(u_2)^2 = u^2 + c(1 - c)w^2 .$$

Using this relation and (22), we can calculate the following

$$\rho'_1 u_1[e_1 + (u_1)^2/2] + \rho'_2 u_2[e_2 + (u_2)^2/2] =$$

$$= \rho\{ u\, e + u^3/2 + u\, c(1 - c)w^2/2 + c(1 - c)w\, [e_1 - e_2 + u\, w + (1 - 2c)w^2/2] \} ,$$

and from (21):

$\rho'_1[e_1 + (u_1)^2/2] + \rho'_2[e_2 + (u_2)^2/2] = \rho\,[\,e + u^2/2 + c(1-c)w^2/2]$.

Finally,

$p'_1 u_1 + p'_2 u_2 = p'_1[u + (1-c)\,w] + p'_2[u - c\,w] =$

$= (p'_1 + p'_2)\,u + w[(1-c)\,p'_1 - c\,p'_2] = p\,u + w\,[\rho'_1(1-c)\,p'_1/\,\rho'_1 - \rho'_2 c\,p'_2/\,\rho'_2] =$

$= p\,u + \rho\,w\,[c(1-c)\,p'_1/\,\rho'_1 - c(1-c)\,p'_2/\,\rho'_2] = p\,u + \rho\,w\,c(1-c)\,[p_1/\,\rho_1 - p_2/\,\rho_2]$.

Let us denote

$$E = e + c(1-c)w^2/2, \tag{24}$$

then the energy conservation equation takes the following form for the two-phase medium:

$$\frac{\partial\rho\left(E + u^2/2\right)}{\partial t} + \frac{\partial\left\{\rho u\left(E + u^2/2\right) + pu + \rho c(1-c)w\left[n + uw + (1-2c)w^2/2\right]\right\}}{\partial x} = 0\,.$$

It is seen that it is convenient to calculate the chemical potential from the specific energy E including the diffusion term:

$\Lambda = E_c = e_1 - e_2 + p_1/\,\rho_1 - p_2/\,\rho_2 + (1-2c)\,w^2/2$.

Then the kinetic equation for the velocity difference (23) takes the following form

$$\frac{\partial w}{\partial t} + \frac{\partial[uw + \Lambda]}{\partial x} = \Psi\,. \tag{25}$$

It can be noticed that $E_w = c(1-c)w$, then the energy conservation takes the following form:

$$\frac{\partial\rho\left(E + u^2/2\right)}{\partial t} + \frac{\partial\left\{\rho u\left(E + u^2/2\right) + pu + \rho uwE_w + \rho E_w\Lambda\right\}}{\partial x} = 0\,. \tag{26}$$

Summarizing, the complete system of equations for a two-phase medium involves equations (13-15), (20), and (25-26):

$$\begin{aligned}
&\frac{\partial\rho}{\partial t}+\frac{\partial\rho u}{\partial x}=0\,,\\
&\frac{\partial\rho u}{\partial t}+\frac{\partial\left[\rho u^2+p+\rho wE_w\right]}{\partial x}=0\,,\\
&\frac{\partial\rho\left(E+u^2/2\right)}{\partial t}+\frac{\partial\left\{\rho u\left(E+u^2/2\right)+pu+\rho uwE_w+\rho E_w\Lambda\right\}}{\partial x}=0\,,\\
&\frac{\partial\rho c}{\partial t}+\frac{\partial\left[\rho uc+\rho E_w\right]}{\partial x}=m_0^*\,,\\
&\frac{\partial\rho\theta}{\partial t}+\frac{\partial\rho u\theta}{\partial x}=\Phi\,,\\
&\frac{\partial w}{\partial t}+\frac{\partial\left[uw+\Lambda\right]}{\partial x}=\Psi\,.
\end{aligned}\tag{27}$$

This is almost identically the system of equations, describing a two-phase medium, which has been obtained in [2]. The system is thermodynamically consistent, because if a generalized equation of state is given in the form

$$E = E\,(\rho, S, c, \theta, w)\,,$$

then the entropy evolution equation can be obtained from (27) and the conditions of hyperbolicity deduced [2]. However, within the formulation [2] there is no a thermodynamic identity specified, which would clearly relate the forces, appearing as $p + \rho w E_w$, to the energy E.

3. Thermodynamic identity

In this section we are reconsidering the model to derive thermodynamic identity and obtain a more convenient system, which could be generalized for the case of multiple phases.

Let us analyze the jump conditions for the system (27). We neglect kinetic rates (the right-hand sides in (27)) for derivation of the conditions. Let us denote the jump velocity by D, and then the jump conditions take the following form:

$$\begin{aligned}
&\rho\,(u-D)=\text{const}\,,\\
&\rho u\,(u-D)+p+\rho wE_w=\text{const}\,,\\
&\rho(E+u^2/2)\,(u-D)+u\,(p+\rho wE_w)+\rho E_w\Lambda=\text{const}\,,\\
&\rho c\,(u-D)+\rho E_w=\text{const}\,,
\end{aligned}\tag{28}$$

$$\rho\theta\,(u - D) = \text{const} \;,$$

$$w\,(u - D) + \Lambda = \text{const} \;.$$

It is well known that for a two-parametric medium (a medium, which can be completely described with two parameters, e.g., density and entropy) the conditions of continuity on the contact jump appear as the equality of pressure and velocity. Here we describe the contact jump as a jump, moving with the medium, i.e., the jump velocity is equal to the fluid velocity. Let us derive similar conditions for the present two-phase medium. If we take $u = D$, then the contact conditions follow from (28) as

$$p + \rho w E_w = \text{const} \;, \quad \rho E_w = \text{const} \;, \quad \Lambda = \text{const} \;. \tag{29}$$

It is seen that the role of pressure play the following functions: $p + \rho w E_w$, ρE_w, and Λ. We suppose that these functions relate directly to the thermodynamic relations of the medium. Let us introduce a generalized pressure:

$$P = p + \rho w E_w \;. \tag{30}$$

It should be noted that replacement of pressure by a combination involving also the diffusive components has been considered in theories of mixture long ago, by Truesdell [3] and many other researchers, as well as introduction of the diffusion terms in the internal energy similarly to (24). A diffusion force for the second relation in (29) could be introduced as

$$\Omega = \rho E_w \;. \tag{31}$$

Thus, the functions, preserved through the contact jump, are P, Λ, and Ω.

A quantity, which does not change through any jump, is mass $m = \rho\,(u - D)$. Then the conditions (28) can be rewritten as

$$m = \text{const} \;, mu + P = \text{const} \;, m(E + u^2/2) + uP + \Lambda\Omega = \text{const} \;,$$

$$mc + \Omega = \text{const} \;, m\theta = \text{const} \;, m(w/\rho) + \Lambda = \text{const} \;.$$

It is seen from these relations that basic variables associated with fluxes of Λ, and Ω are mass concentration c and w/ρ. Therefore, it is convenient to introduce a new variable (a specific diffusion velocity):

$$v = w/\rho \;. \tag{32}$$

Now from (24) we can see that

$$E = e(\rho, S, c, \theta) + \rho^2 c(1 - c)v^2/2 \;, \tag{33}$$

and the function Ω is calculated as $\Omega = E_v$. The function Λ can be calculated as above in accordance with $\Lambda = E_c$. However, what is even more important, the generalized pressure can be calculated via E as $P = \rho^2 E_\rho$. The specific energy also depends on θ, so we have to introduce a function $\Pi = E_\theta$. From (9) it can be found

$$\Pi = c(e_1)_{\rho 1}(\rho c/\theta)_\theta + (1-c)(e_2)_{\rho 2}(\rho(1-c)/(1-\theta))_\theta =$$

$$= -(\rho_1)^2(e_1)_{\rho 1}/\rho + (\rho_2)^2(e_2)_{\rho 2}/\rho = -(p_1 - p_2)/\rho \,.$$

Putting those equations together, we have:

$$T = E_S \;,\quad P = \rho^2 E_\rho \;,\quad \Lambda = E_c \;,\quad \Omega = E_v \;,\quad \Pi = E_\theta \,. \tag{34}$$

Thus, the following thermodynamic identity takes place

$$T\,\mathrm{d}S = \mathrm{d}E + P\,\mathrm{d}V - \Lambda\,\mathrm{d}c - \Omega\,\mathrm{d}v - \Pi\,\mathrm{d}\theta \,. \tag{35}$$

The system (27) can be rewritten in the following form

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0\,,\\
&\frac{\partial \rho u}{\partial t} + \frac{\partial\left[\rho u^2 + P\right]}{\partial x} = 0\,,\\
&\frac{\partial \rho\left(E + u^2\!/_2\right)}{\partial t} + \frac{\partial\left\{\rho u\left(E + u^2\!/_2\right) + Pu + \Lambda\Omega\right\}}{\partial x} = 0\,,\\
&\frac{\partial \rho c}{\partial t} + \frac{\partial\left[\rho u c + \Omega\right]}{\partial x} = m_0^*\,,\\
&\frac{\partial \rho\theta}{\partial t} + \frac{\partial \rho u\theta}{\partial x} = \Phi\,,\\
&\frac{\partial \rho v}{\partial t} + \frac{\partial\left[\rho u v + \Lambda\right]}{\partial x} = \Psi\,.
\end{aligned} \tag{36}$$

Concluding, selection of the potential in the form

$$E = E\,(\rho, S, c, \theta, v) \tag{37}$$

along with the identity (35) closes the model (36). In fact, the potential E can be calculated as earlier, using (33) and (9) along with the local equations of state (19).

4. Model of multi-phase flows

In the present section we shall follow more traditional denotations, being used in the mixture theories (e.g., [3]), which are associated with the centre mass velocity and diffusion velocities. This choice is sometimes more convenient because it is not associated with a specific component of a mixture and treats the mixture components equally. Thus, for a n-phase medium we denote c_i as mass concentration of i-th component of the mixture (i=1, … , n). We suppose that the multi-phase medium has n components and summation from i=1 up to i= n will be denoted by sign Σ. As usual, $c_i = m_i/m$, where m_i is the mass fraction of the i-th component in the volume V of mass m. Similarly, $\theta_i = V_i/V$ that gives $\Sigma c_i = 1$ and $\Sigma \theta_i = 1$. At the moment we ignore the interdependence of the variable sets c_i and θ_i at i=1, … , n; we will recall this fact at the end of the section when this interdependence is relevant. We introduce average velocity u exactly how we have done it in the previous section:

$$u = \Sigma c_i u_i \ . \tag{38}$$

However, to preserve universality, we define the velocity nonequilibrium in a different manner in accordance with the traditional choice of diffusion velocities, which is proportional to the well-known diffusion fluxes $\rho_i(u_i - u)$:

$$w_i = u_i - u \ . \tag{39}$$

It can be noted that, comparing this choice with the choice in the previous section, the diffusion velocities would be $w_1 = u_1 - u = (1-c)\, w$ and $w_2 = u_2 - u = -c\, w$. It follows $cw_1+(1-c)\, w_2 = 0$, or, generally:

$$\Sigma c_i w_i = 0 \, . \tag{40}$$

The diffusion velocity interdependence will also be ignored at the moment. Keeping in mind the results of the preceding section, we select the following variables as the basic ones:

$$\rho,\ S,\ u,\ c_i,\ \theta_i,\ v_i. \tag{41}$$

Again, the variables are independent at i=1,…,n-1, but at the moment we consider the overdetermined set (41) at i=1,…,n. The local densities are, similar to (8):

$$\rho_i = \rho\, c_i/\theta_i \ . \tag{42}$$

From (39) $u_i = u + \rho v_i$, that allows us to determine the kinetic equations for c_i:

$$\frac{\partial \rho c_i}{\partial t} + \frac{\partial(\rho u c_i + \Omega_i)}{\partial x} = \dot{m}_i \ , \tag{43}$$

here $\Omega_i = \rho^2 c_i v_i = \rho c_i w_i$ ($\Sigma\, \Omega_i = 0$ from (40)) and m^*_i is the mass exchange rate such that $\Sigma m^*_i = 0$, when assuming that for the i-th phase the equations are chosen in the form identical to (1) replacing the subscript index '1' by 'i'. Summing up the continuity equations of (1), we have the continuity equation for the mixture coincident with (13):

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0 . \tag{44}$$

The volumetric concentrations behave similarly, regardless of the number of phases:

$$\frac{\partial \rho \theta_i}{\partial t} + \frac{\partial \rho u \theta_i}{\partial x} = \Phi_i . \tag{45}$$

Let us define a generalized internal energy of i-th phase, invoking the diffusion energy:

$$E_i = e_i + w_i^2/2 = e_i + \rho^2 v_i^2/2 . \tag{46}$$

The mass averaging of (46) gives the energy of the mixture, similarly to (33):

$$E = \Sigma\, c_i E_i = e + \Sigma\, c_i w_i^2/2 = e + \rho^2 \Sigma\, c_i v_i^2/2 , \tag{47}$$

here $e = \Sigma\, c_i e_i$. Differentiating E over ρ, we obtain generalized pressure similarly to (30):

$$P = \rho^2 E_\rho = \rho^2 e_\rho + \rho^3 \Sigma\, c_i v_i^2 = \rho^2 e_\rho + \rho\, \Sigma\, c_i w_i^2 = p + \rho\, \Sigma\, c_i w_i^2 , \tag{48}$$

where pressure can be treated as in the preceding section: $p = \Sigma\, p'_i = \Sigma\, \theta_i p_i$. For derivation of the momentum and energy equations for the mixture we need several auxiliary relations:

$$\begin{aligned}
&\Sigma\, c_i u_i^2 = u^2 + \Sigma\, c_i w_i^2 , \\
&\Sigma\, \rho c_i (e_i + u_i^2/2) = \rho\, (e + u^2/2 + \Sigma\, c_i w_i^2/2) , \\
&\Sigma\, u_i p'_i = up + \rho\, \Sigma\, c_i w_i\, p_i/\rho_i , \\
&\Sigma\, \rho c_i u_i\, (e_i + u_i^2/2) = \rho u\, (e + u^2/2 + \Sigma\, c_i w_i^2/2) + \rho u\, \Sigma\, c_i w_i^2 + \rho\, \Sigma\, c_i w_i e_i + \rho\, \Sigma\, c_i w_i^3/2 .
\end{aligned} \tag{49}$$

Summing up the momentum equations in the form (1), we obtain an equation similar to (20) with the generalized pressure from (48):

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \left(\rho u^2 + P\right)}{\partial x} = 0 . \tag{50}$$

When summing up, we have to use the momentum balance in the form $\Sigma n^*_i = 0$. To derive the kinetic equation for the diffusion velocity, we rewrite the momentum equation in the following form

$$\frac{\partial u_i}{\partial t} + u_i \frac{\partial u_i}{\partial x} + \frac{1}{\rho_i'} \frac{\partial p_i'}{\partial x} = \left(n_i^* - m_i^* u_i\right)/\rho_i' \,, \tag{51}$$

and the equation (50) in the similar form

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial P}{\partial x} = 0 \,. \tag{52}$$

Using $\mathrm{d}\,(e_i + p_i/\rho_i) = \mathrm{d}p'_i/\rho'_i$, $\mathrm{d}\,(E + P/\rho) = \mathrm{d}P/\rho$ and an analogue of (22) in the form $u_i^2 - u^2 = 2uw_i + w_i^2$, we can derive the required equation by subtracting (51) from (52):

$$\frac{\partial w_i}{\partial t} + \frac{\partial\left(uw_i + w_i^2/2\right)}{\partial x} + \frac{\partial}{\partial x}\left(e_i + \frac{p_i}{\rho_i} - E - \frac{P}{\rho}\right) = \left(n_i^* - m_i^* u_i\right)/\rho_i' = \Psi_i \,.$$

Let us introduce a chemical potential as follows

$$\Lambda_i = E_i + \frac{p_i}{\rho_i} - E - \frac{P}{\rho} = e_i + \frac{w_i^2}{2} + \frac{p_i}{\rho_i} - E - \frac{P}{\rho} \quad . \tag{53}$$

For future references a part of the potential, which is not related to a specific phase will be denoted by $\Lambda_0 = E + P/\rho$. Then the equation for specific diffusion velocity takes its final form

$$\frac{\partial \rho v_i}{\partial t} + \frac{\partial\left(\rho u v_i + \Lambda_i\right)}{\partial x} = \Psi_i \,. \tag{54}$$

The effect of change in volumetric concentration onto the specific energy is taken into account by introduction of Π_i, similarly to that in the second section:

$$\Pi_i = E_{\theta i} = c_i(e_i)_{\theta i} = c_i(e_i)_{\rho i}(\rho_i)_{\theta i} = -\, c_i(e_i)_{\rho i}(\rho\, c_i/\theta_i^2) = -\, p_i/\rho \quad . \tag{55}$$

Finally, the energy equation is derived by summation of the energy conservation laws in the form (1) and use of (49):

$$\frac{\partial \rho\left(E + u^2/2\right)}{\partial t} + \frac{\partial\left[\rho u\left(E + u^2/2\right) + Pu + \rho \Sigma c_i w_i\left(e_i + w_i^2/2 + p_i/\rho_i\right)\right]}{\partial x} = 0 \,.$$

One more relation is necessary for finalizing the derivation of the energy conservation equation:

$\rho\, \Sigma\, c_i w_i\, (e_i + w_i^2/2 + p_i/\rho_i) = \Sigma\, \rho c_i w_i\, (e_i + w_i^2/2 + p_i/\rho_i - \Lambda_0) = \Sigma\, \Omega_i \Lambda_i$,

here we used definitions of Ω_i and Λ_i, and $\Sigma\, \Omega_i = 0$. Finally, the energy equation takes the following final form

$$\frac{\partial \rho\left(E + {u^2}/{2}\right)}{\partial t} + \frac{\partial\left[\rho u\left(E + {u^2}/{2}\right) + Pu + \Sigma \Lambda_i \Omega_i\right]}{\partial x} = 0 . \tag{56}$$

The complete system of equations, generalising (36), combines (43-45), (50), (54), (56) into the following

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0 , \\
&\frac{\partial \rho u}{\partial t} + \frac{\partial\left(\rho u^2 + P\right)}{\partial x} = 0 , \\
&\frac{\partial \rho\left(E + {u^2}/{2}\right)}{\partial t} + \frac{\partial\left[\rho u\left(E + {u^2}/{2}\right) + Pu + \Sigma \Lambda_i \Omega_i\right]}{\partial x} = 0 , \\
&\frac{\partial \rho c_i}{\partial t} + \frac{\partial\left(\rho u c_i + \Omega_i\right)}{\partial x} = m_i^* , \\
&\frac{\partial \rho \theta_i}{\partial t} + \frac{\partial \rho u \theta_i}{\partial x} = \Phi_i , \\
&\frac{\partial \rho v_i}{\partial t} + \frac{\partial\left(\rho u v_i + \Lambda_i\right)}{\partial x} = \Psi_i .
\end{aligned} \tag{57}$$

Concluding the section, we can write out the thermodynamic identity for the multi-phase mixture:

$$T\, \mathrm{d}S = \mathrm{d}E + P\, \mathrm{d}V - \Sigma\, (\Lambda_i + \Lambda_0)\mathrm{d}c_i - \Sigma\, \Omega_i\, \mathrm{d}v_i - \Sigma\, \Pi_i\, \mathrm{d}\theta_i\ , \tag{58}$$

which provides us with the closure relations:

$$T = E_S\ ,\quad P = \rho^2 E_\rho\ ,\quad \Lambda_i + \Lambda_0 = E_{ci}\ ,\quad \Omega_i = E_{vi}\ ,\quad \Pi_i = E_{\theta i}\ . \tag{59}$$

For completeness we have to calculate the function Λ_0 in the following way

$$\Sigma\, c_i E_{ci} = \Sigma\, c_i(e_i + w_i^2/2 + p_i/\rho_i) = \Sigma\, c_i(e_i + w_i^2/2 + \theta_i p_i/(c_i \rho)) = E + p/\rho =$$

$$= E + (P - \rho\, \Sigma\, c_i w_i^2)/\rho = \Lambda_0 - \rho^2 \Sigma\, c_i v_i^2\ ,$$

that is

$$\Lambda_0 = \Sigma\, c_i(E_{ci} + \rho^2 v_i^2) \ . \tag{60}$$

Regarding the entry of the function Λ_0 in the identity (58), we notice that the summation is conducted from 1 up to n, so one of the variables is dependent. For example, we can select the n-th mass concentration variable c_n to be expressed via the preceding ones, such as

$$c_n = 1 - c_1 - \ldots - c_{n-1} \ . \tag{61}$$

It should be noted that any of these n variables can be selected dependent on other n–1 ones simply by renumbering and assigning the number n to the pre-selected dependent one. Then the first sum in (58) can be rewritten in the form, containing only the first n–1 independent variables:

$$\Sigma\, (\Lambda_i + \Lambda_0)\mathrm{d}c_i = \Sigma'\, (\Lambda_i - \Lambda_n)\ , \tag{62}$$

where Σ' is the summation sign from 1 up to n–1. Thus, the relation eventually allows us to exclude the function Λ_0 from the consideration.

Finally, we shall show that the closed system, containing only n–1 independent variables, is also thermodynamically consistent. To do this, we select, as for the derivation of (61), that the n-th variables c_n, θ_n, and v_n are dependent on the rest of the set (41). Namely, from (40), (61), and from the similar relation for θ we have

$$c_n = 1 - \Sigma' c_i \ , \quad \theta_n = 1 - \Sigma'\theta_i \ , \quad c_n v_n = -\,\Sigma' c_i v_i \ . \tag{63}$$

Scalar functions in the identity (58) are not affected by the dependencies (63), so the relations

$$T = E_S \ , \quad P = \rho^2 E_\rho$$

are intact. For the next terms in the identity we are conducting separate analyses. The first one concerns $\Sigma\, (\Lambda_i + \Lambda_0)\mathrm{d}c_i$, which is reduced to $\Sigma'\, (\Lambda_i - \Lambda_n)$, according to (62). According to (63), increment in c_i is also involved in the change of v_n. Therefore, for this analysis we have to expand the term $\Sigma\, \Omega_i\, \mathrm{d}v_i$ as well:

$$\Sigma\, \Omega_i\, \mathrm{d}v_i = \Sigma'\, \Omega_i\, \mathrm{d}v_i + \Omega_n\, \mathrm{d}v_n \ . \tag{64}$$

From (63) $\mathrm{d}(c_n v_n) = -\,\Sigma'\mathrm{d}\,(c_i v_i)$ and $\mathrm{d}c_n = -\,\Sigma'\mathrm{d}c_i$ that give

$$v_n \mathrm{d}c_n + c_n \mathrm{d}v_n = c_n \mathrm{d}v_n - v_n \Sigma'\mathrm{d}c_i = -\,\Sigma' v_i \mathrm{d}c_i - \Sigma' c_i \mathrm{d}v_i$$

and

$$c_n dv_n = -\Sigma'(v_i - v_n)dc_i - \Sigma' c_i dv_i \quad . \tag{65}$$

From (63) and (64) it follows

$$\begin{aligned}\Sigma\, \Omega_i\, dv_i &= \Sigma'\, \Omega_i\, dv_i - (\Omega_n/c_n)\, [\Sigma'(v_i - v_n)dc_i + \Sigma' c_i dv_i\,] = \\ &= \Sigma'[\Omega_i - (\Omega_n/c_n)c_i]\, dv_i - (\Omega_n/c_n)\, \Sigma'(v_i - v_n)dc_i \quad .\end{aligned} \tag{66}$$

Thus, according to (62) and (66), the term, associated with the change in c_i in the identity (58) is actually

$$\Lambda_i - \Lambda_n - (\Omega_n/c_n)\,(v_i - v_n) \quad . \tag{67}$$

We have to check out if this term is coincident with E_{ci}. Turning to (42) and (63), c_i is involved in ρ_i, c_n and v_n; differentiating (47) over c_i with this in mind and using (65), we have

$$\begin{aligned}E_{ci} &= E_i + c_i(e_i)_{\rho i}(\rho_i)_{ci} + E_n(c_n)_{ci} + c_n(e_i)_{\rho n}(\rho_n)_{cn}(c_n)_{ci} + c_n(E_n)_{vn}(E_i)_{vi}\,/\,c_n = \\ &= E_i + \rho_i(e_i)_{\rho i} - E_n - \rho_n(e_n)_{\rho n} - \Omega_n\,(v_i - v_n)/c_n = \Lambda_i - \Lambda_n - (\Omega_n/c_n)\,(v_i - v_n) \;,\end{aligned}$$

which is actually coincident with (67). Next stage involves analysis of the term with increment in v_i; this increment appears only in the term (66) and is equal to $\Omega_i - (\Omega_n/c_n)c_i$. We have to check out if it is coincident with E_{vi}. The variable v_i is involved only in v_n; differentiating (47) over v_i and using (65), we can obtain

$$E_{vi} = (E_i)_{vi} + (E_n)_{vn}(v_n)_{vi} = \Omega_i - \Omega_n(c_i/c_n)$$

that is identical to $\Omega_i - (\Omega_n/c_n)c_i$. The last analysis involves the term of (58) with $d\theta_i$; taking into account the interdependence of θ_i in (63), the last term (58) is transformed as follows

$$\Sigma\, \Pi_i\, d\theta_i = \Sigma'\, \Pi_i\, d\theta_i + \Pi_n\, d\theta_n = \Sigma'\, (\Pi_i - \Pi_n)d\theta_i \quad .$$

For the set of independent variables θ_i we have to find out if $\Pi_i - \Pi_n$ is equal to $E_{\theta i}$. To do this, we again differentiate (47) over θ_i:

$$E_{\theta i} = c_i(E_i)_{\theta i} + c_n(E_n)_{\theta n}(\theta_n)_{\theta i} = c_i(e_i)_{\theta i} - c_n(e_n)_{\theta n} = \Pi_i - \Pi_n \quad .$$

This concludes the analysis and proves that for the set of independent variables (41) at i=1,…,n-1 the identity can be written out in the following form

$$\begin{aligned}T\, dS &= dE + P\, dV - \\ &- \quad \Sigma'[\Lambda_i - \Lambda_n - (\Omega_n/c_n)(v_i - v_n)]\, dc_i -\end{aligned} \tag{68}$$

$- \quad \Sigma'[\Omega i - \Omega n\,(ci/cn)]\, dvi - \Sigma'\,(\Pi i - \Pi n)\, d\theta i \quad .$

Keeping the choice of the set of independent variables, the next section is devoted to analysis if this set can be used for construction of conservation laws and kinetic equations similar to (57).

5. Model of multi-phase flows with independent variables

Now, when existence of a single thermodynamic potential is obvious, we shall try to formulate the model, which would involve the independent variables only. We select the set of variables (41) at i=1,...,n-1. We have to rewrite the specific internal energy applicable to the present case. From (47) and (63) it follows

$$E = \Sigma\, c_i E_i = \Sigma\, c_i e_i + \rho^2 \Sigma\, c_i v_i^2/2 = \Sigma' c_i e_i + c_n e_n + (\rho^2/2)\, \Sigma c_i v_i^2 =$$

$$= \Sigma' c_i (e_i - e_n) + e_n + (\rho^2/2) \Sigma c_i v_i^2 \quad . \qquad (69)$$

Turning to the system (57), it is obvious, that the mass and momentum conservation equations do not suffer any changes associated with the choice of independent variables. The energy equation contains the following term $\Sigma\Lambda_i\Omega_i$, which changes with the new choice of variables. With the use of $\Sigma\, \Omega_i = 0$, this term is transformed as follows:

$$\Sigma\, \Lambda_i\Omega_i = \Sigma'\Lambda_i\Omega_i + \Lambda_n\Omega_n = \Sigma'\Lambda_i\Omega_i - \Lambda_n\, \Sigma'\Omega_i = \Sigma'\, \Omega_i(\Lambda_i - \Lambda_n) \quad . \qquad (70)$$

It is seen that use of the function $\Lambda_i - \Lambda_n$ is preferable in the present case. For this function to be involved, we have to modify equations for the specific diffusion velocity by subtraction of the last one from the rest of them at i=1,...,n-1. We introduce a new variable, which is a relative diffusion velocity v'_i, as $v'_i = v_i - v_n$. Then the kinetic equations for v'_i follow directly from (57):

$$\frac{\partial \rho v_i'}{\partial t} + \frac{\partial\left(\rho u v_i' + \Lambda_i'\right)}{\partial x} = \Psi_i' \, . \qquad (71)$$

Here $\Lambda'_i = \Lambda_i - \Lambda_n$ and $\Psi'_i = \Psi_i - \Psi_n$. Let us calculate a sum of the diffusion terms in (69), using a new notation for the relative diffusion velocity and (63):

$$\Sigma c_i v_i = \Sigma' c_i v_i + c_n v_n = \Sigma' c_i v_i + (1 - \Sigma' c_i)\, v_n = \Sigma' c_i (v_i - v_n) + v_n = \Sigma' c_i v'_i + v_n = 0 \ ,$$

$$v_n = - \Sigma' c_j v'_j \ ,$$

$$v_i = v'_i + v_n = v'_i - \Sigma' c_j v'_j \quad , \qquad (72)$$

$$\Sigma c_i v_i^2 = \Sigma' c_i v_i^2 + c_n v_n^2 = \Sigma' c_i (v'_i - \Sigma' c_j v'_j)^2 + (1 - \Sigma' c_i)(\Sigma' c_j v'_j)^2 =$$

$$= \Sigma' c_i (v'_i)^2 - 2\,(\Sigma' c_i\, v'_i)(\Sigma' c_j v'_j) + (\Sigma' c_i)(\Sigma' c_j v'_j)^2 + (\Sigma' c_j v'_j)^2 -$$

$$- (\Sigma' c_i)(\Sigma' c_j v'_j)^2 = \Sigma' c_i (v'_i)^2 - (\Sigma' c_j v'_j)^2 \ .$$

Thus, the set of independent variables (41) is transformed into

$$\rho,\ S,\ u,\ c_i,\ \theta_i,\ v'_i, \quad i=1,\dots,n-1. \tag{73}$$

Using (71), the system (57) takes the following form:

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0\,, \\
&\frac{\partial \rho u}{\partial t} + \frac{\partial \left(\rho u^2 + P\right)}{\partial x} = 0\,, \\
&\frac{\partial \rho \left(E + u^2/2\right)}{\partial t} + \frac{\partial \left[\rho u \left(E + u^2/2\right) + Pu + \Sigma' \Lambda'_i \Omega_i\right]}{\partial x} = 0\,, \\
&\frac{\partial \rho c_i}{\partial t} + \frac{\partial \left(\rho u c_i + \Omega_i\right)}{\partial x} = m_i^*\,, \\
&\frac{\partial \rho \theta_i}{\partial t} + \frac{\partial \rho u \theta_i}{\partial x} = \Phi_i\,, \\
&\frac{\partial \rho v'_i}{\partial t} + \frac{\partial \left(\rho u v'_i + \Lambda'_i\right)}{\partial x} = \Psi'_i\,,
\end{aligned} \tag{74}$$

at $i=1,\dots,n-1$. With the formula (72) the specific energy (69) is written out as follows

$$E = \Sigma' c_i (e_i - e_n) + e_n + (\rho^2/2)[\Sigma' c_i (v'_i)^2 - (\Sigma' c_j v'_j)^2] \ . \tag{75}$$

Finally, we have to adjust the thermodynamic identity (68) to the variables (73). It is clear that the equations $T = E_S$ and $P = \rho^2 E_\rho$ preserve their form because the transformation does not touch scalar variables. Let us differentiate the specific energy (73) over the variables c_i, θ_i, and v'_i. When differentiating over c_i and using (63), we have

$$E_{ci} = e_i - e_n + c_i (e_i)_{\rho i} (\rho_i)_{ci} + c_n (e_n)_{\rho n} (\rho_n)_{cn}\, (c_n)_{ci} + (\rho^2/2)[(v'_i)^2 - 2\,(\Sigma' c_j v'_j) v'_i] =$$

$$= e_i - e_n + \rho_i (e_i)_{\rho i} - \rho_n (e_n)_{\rho n} + (\rho^2/2)\, v'_i\, [v'_i + 2 v_n] =$$

$$= e_i - e_n + p_i/\rho_i - p_n/\rho_n + \rho^2 (v_i^2 - v_n^2)/2 \ ,$$

which is exactly $\Lambda_i - \Lambda_n = \Lambda'_i$ from (53). Let us differentiate E over θ_i and use (63):

$E_{\theta i} = c_i(e_i)_{\rho i}(\rho_i)_{\theta i} + c_n(e_n)_{\rho n}(\rho_n)_{\theta n}(\theta_n)_{\theta i} = -p_i/\rho + p_n/\rho$.

Thus, the function Π_i in (59) has to be transformed into

$$\Pi'_i = \Pi_i - \Pi_n \ . \tag{76}$$

The last step is differentiation of E in (75) over v'_i with the use of (72):

$$E_{v'i} = \rho^2 [\, c_i v'_i - (\Sigma' c_j v'_j)\cdot c_i] = \rho^2 c_i\, [v'_i - \Sigma' c_j v'_j] = \rho^2 c_i\, v_i \quad . \tag{77}$$

It is seen from (43) that $E_{v'i}$ is exactly coincident with Ω_i.

Thus, the thermodynamic identity can be easily written out for the present case:

$$T\,\mathrm{d}S = \mathrm{d}E + P\,\mathrm{d}V - \Sigma'\Lambda'_i\,\mathrm{d}c_i - \Sigma'\Omega_i\,\mathrm{d}v'_i - \Sigma'\Pi'_i\,\mathrm{d}\theta_i \ . \tag{78}$$

Thus, if the potential E is given, the functions involved in the system (74) are explicitly calculated with the help of the identity (78).

It is interesting to note that the present case is directly reducible to the case of the two-phase media at n=2 derived in the third section because $w = v'_1$, and $\Lambda = \Lambda'_1$ and $\Omega = \Omega'_1$.

The identity (78) gives us the rules for calculation of the functions entering (74) via the potential $E(\rho, S, c_i, \theta_i, v'_i)$:

$$T = E_S \ , \quad P = \rho^2 E_\rho \ , \quad \Lambda'_i = E_{ci} \ , \quad \Omega_i = E_{v'i} \ , \quad \Pi'_i = E_{\theta i} \ . \tag{79}$$

Expanding the energy equation in (74) and applying (79), we can obtain the following entropy evolution equation:

$$\rho T \frac{dS}{dt} = -\Sigma'\Lambda'_i m_i^* - \Sigma'\Pi'_i \Phi_i - \Sigma'\Omega_i \Psi'_i \quad , \tag{80}$$

here $d/dt = \partial/\partial t + \mathrm{u}\cdot\partial/\partial x$ is the particle derivative. Using (80), the correctness requires the following entropy nondecreasing condition to be satisfied:

$$-\Sigma'\Lambda'_i m^*_i - \Sigma'\Pi'_i\Phi_i - \Sigma'\Omega_i\Psi'_i \geq 0 \ . \tag{81}$$

An equivalent condition could also be derived from the overdetermined system (57), (58):

$$\rho T \frac{dS}{dt} = -\Sigma\Lambda_i m_i^* - \Sigma\Pi_i \Phi_i - \Sigma\Omega_i \Psi_i \quad , \tag{82}$$

here relations $\Sigma\,\Omega_i = 0$ and $\Sigma\, m^*_i = 0$ have been used. It is interesting to note that for the choice of kinetic relations suggested in [2] as $m^*_i = 0$, $\Phi_i = -\rho\Pi_i/\tau$, $\Psi_i = -\kappa\Omega_i$, the entropy nondecreasing condition is satisfied automatically. Moreover, the Onsager principle [9] is satisfied, because the quadratic form $\rho\Sigma\,(\Pi_i)^2/\tau + \kappa\Sigma\,(\Omega_i)^2$, appearing for this case as the right-hand side in (82), is symmetrical.

6. Hyperbolicity of the two-phase model

In this section we analyse eigenvalues of the system (36). Hyperbolicity of the prototype system (27) has been considered in [2] and the eigenvalues have been calculated for the case of absence of diffusivity ($w = 0$). To analyse the system (36) we shall rewrite it in the following form, replacing the energy conservation law with the entropy evolution equation (similar to the equation (80) for the case of two phases):

$$
\begin{aligned}
&\frac{d\rho}{dt} + \rho\frac{\partial u}{\partial x} = 0\,,\\
&\frac{du}{dt} + \frac{P_\rho}{\rho}\frac{\partial \rho}{\partial x} + \frac{P_c}{\rho}\frac{\partial c}{\partial x} + \frac{P_\theta}{\rho}\frac{\partial \theta}{\partial x} + \frac{P_v}{\rho}\frac{\partial v}{\partial x} + \frac{P_S}{\rho}\frac{\partial S}{\partial x} = 0\,,\\
&\frac{dc}{dt} + \frac{\Omega_\rho}{\rho}\frac{\partial \rho}{\partial x} + \frac{\Omega_c}{\rho}\frac{\partial c}{\partial x} + \frac{\Omega_\theta}{\rho}\frac{\partial \theta}{\partial x} + \frac{\Omega_v}{\rho}\frac{\partial v}{\partial x} = 0\,,\\
&\frac{d\theta}{dt} = 0\,,\\
&\frac{dS}{dt} = 0\,,\\
&\frac{dv}{dt} + \frac{\Lambda_\rho}{\rho}\frac{\partial \rho}{\partial x} + \frac{\Lambda_c}{\rho}\frac{\partial c}{\partial x} + \frac{\Lambda_\theta}{\rho}\frac{\partial \theta}{\partial x} + \frac{\Lambda_v}{\rho}\frac{\partial v}{\partial x} + \frac{\Lambda_S}{\rho}\frac{\partial S}{\partial x} = 0\,,
\end{aligned}
\qquad (83)
$$

here $d/dt = \partial/\partial t + u\cdot\partial/\partial x$ – is the particle derivative, and we have neglected the right-hand sides, because they do not affect the characteristic behaviour of the system. The system can in general be written out in the following matrix form:

$$
\frac{\partial U}{\partial t} + A\frac{\partial U}{\partial x} = 0\,, \qquad (84)
$$

where $U = \{\rho, u, c, \theta, s, v\}$, and A is matrix of coefficients of the system (83). As a result, the characteristic equation of the system $\det(A - \lambda I) = 0$ for eigenvalues λ is specified to the following characteristic determinant:

$$\det\left(\begin{array}{c|c|c|c|c|c} \chi & \rho & 0 & 0 & 0 & 0 \\ \hline P_\rho/\rho & \chi & P_c/\rho & P_\theta/\rho & P_s/\rho & P_v/\rho \\ \hline \Omega_\rho/\rho & 0 & \chi' & \Omega_\theta/\rho & 0 & \Omega_v/\rho \\ \hline 0 & 0 & 0 & \chi & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \chi & 0 \\ \hline \Lambda_\rho/\rho & 0 & \Lambda_c/\rho & \Lambda_\theta/\rho & \Lambda_v/\rho & \chi' \end{array}\right) = 0 \quad , \tag{85}$$

where $\chi = u - \lambda$ and $\chi' = \chi + e_0$, $e_0 = E_{vc}/\rho$. Expanding (85), the characteristic polynomial takes the following form

$$\chi^2\left\{\chi^2\left(\chi'^2 - \frac{1}{\rho^2}\Lambda_c\Omega_v\right) - \rho\left[\frac{1}{\rho}P_\rho\chi'^2 + \frac{1}{\rho^3}P_c\Omega_v\Lambda_\rho + \frac{1}{\rho^3}P_v\Omega_\rho\Lambda_c - \right.\right.$$
$$\left.\left. - \frac{1}{\rho^2}P_v\Lambda_\rho\chi' - \frac{1}{\rho^3}P_\rho\Omega_v\Lambda_c - \frac{1}{\rho^2}P_c\Omega_\rho\chi'\right]\right\} = 0\,. \tag{86}$$

Combining the first and fifth terms in the square parentheses and memorizing the zero double root $\chi = 0$, the polynomial for the rest four roots is reduced to the following

$$\left(\chi^2 - P_\rho\right)\left(\chi'^2 - \frac{1}{\rho^2}\Lambda_c\Omega_v\right) -$$
$$- \rho\left(\frac{1}{\rho^3}P_c\Omega_v\Lambda_\rho + \frac{1}{\rho^3}P_v\Omega_\rho\Lambda_c - \frac{1}{\rho^2}P_v\Lambda_\rho\chi' - \frac{1}{\rho^2}P_c\Omega_\rho\chi'\right) = 0\,. \tag{87}$$

Let us introduce the following denotations:

$$\mathrm{A} = E_{\rho c}\,, \quad \mathrm{B} = E_{\rho v}\,, \quad \Theta_1 = E_{cc}/\rho\,, \quad \Theta_2 = E_{vv}/\rho\,, \quad l^2 = P_\rho\,. \tag{88}$$

Then, from the consequence (34) of the thermodynamic identity we can obtain

$$\Lambda_\rho = \mathrm{A}\,, \quad P_c = \rho^2\mathrm{A}\,, \quad \Omega_\rho = \mathrm{B}\,, \quad P_v = \rho^2\mathrm{B}\,, \quad \Lambda_c/\rho = \Theta_1\,, \quad \Omega_v/\rho = \Theta_2\,. \tag{89}$$

We use the following denotations throughout the section $l^2 = P_\rho$ and $k^2 = \Theta_1 \cdot \Theta_2$. It is assumed that P_ρ, Θ_1 and Θ_2 are positive. That gives us the following set of conditions in terms of the equation of state

$$(\rho^2 E_\rho)_\rho > 0\,, \quad E_{cc} > 0\,, \quad E_{vv} > 0\,. \tag{90}$$

Then the characteristic equation takes the following form:

$$F(\chi)=(\chi^2-l^2)(\chi'^2-\Theta_1\cdot\Theta_2)+2\rho AB\chi'-\rho(A^2\Theta_2+B^2\Theta_1)=0\,. \tag{91}$$

With use of (9), (24) and (88) we can calculate one of the coefficients:

$$A\cdot B=\rho v(k^2-l^2+\rho^2v^2)\quad . \tag{92}$$

It can be straightforward checked out that the polynomial is exactly coincident with the one derived in [2]. The present polynomial has a simpler form just because of the term reduction associated with the generalization of pressure and energy; the present generalization contributes in additional terms related to the density derivatives of the diffusion components which are involved in the characteristic polynomial of [2] as a separate term. It has been shown in [2] that roots of the characteristic polynomial are real in the vicinity of a state with $w = 0$ ($v = 0$ for the present model). In fact, this state gives B = 0 and $e_0 = 0$, resulting in the following bi-quadratic equation

$$(\chi^2-l^2)(\chi^2-k^2)-\rho A^2\Theta_2=0\ .$$

The present simpler form of the characteristic polynomial allows us to assess the hyperbolicity of the model in a wider range of parameters. To study the polynomial roots we will check the number of sign changes. Firstly, we rewrite the polynomial in a form, which is more convenient for the analysis employing new variable $z = \chi + e_0/2$. Expanding (91) with help of (92), we can obtain the equation for z:

$$P(z)=z^4-2p\cdot z^2+2q\cdot z+r=0\ , \tag{93}$$

where

$$p=(k^2+l^2+e_0^2/2)/2\ ,$$

$$q=(k^2-l^2)\cdot e_0/2+\rho^2v\cdot(k^2-l^2+\rho^2v^2)\quad ,$$

$$r=k^2\cdot l^2-(k^2+l^2-e_0^2/4)\cdot e_0^2/4+(k^2-l^2+\rho^2v^2)\cdot\rho^2v\cdot e_0-\rho(A^2\Theta_2+B^2\Theta_1)\quad .$$

It is obvious that the polynomial (93) has the positive sign at large enough negative and positive values of z. If we show that the polynomial is negative at two certain points and has the positive sign at a point between the two then it means that the polynomial has four real roots. We choose the following three points:

$$z_-=-p^{1/2}\,,\quad z_+=p^{1/2}\ ,\quad z_0=q/p\quad .$$

Then from (93):

$$P(z_-)=-p^2-2qp^{1/2}+r\ ,$$

$$P(z_+)=-p^2+2qp^{1/2}+r\ ,$$

$P(z_0) = q^4/p^4 + r$.

If we demand that $P(z_-) < 0$, $P(z_+) < 0$ and $P(z_0) > 0$ then the polynomial (91) will have four real roots. To satisfy these conditions it is sufficient that

$$r > 0 \ , \qquad p^2 > r + 2|q|p^{1/2} \ . \tag{94}$$

When the denotations in (94) having been decoded with (88)-(89), these conditions (94) along with (90) give necessary conditions of existence of 4 roots of the characteristic polynomial (91). When the generalized specific energy E is specified, the conditions (94) can be straightforward checked out. The values z_-, z_+, and z_0 can be used for the root separation. The estimate (94) is not the best possible one; for instance, choice of q/(2p) as z_0 would give less restrictive assessment for the coefficient r in (94). However, the conditions (94) demonstrate that there is a fairly wide range of parameters, which guarantee existence of real roots of the characteristic polynomial.

7. Discussion and Conclusion

A model for multi-phase flows has been built up and the thermodynamic identity derived, allowing us to close the model with a single thermodynamic potential - a generalized specific energy E. In doing so, a link between the generalized pressure and energy, involving the diffusion terms, has been established for the one-dimensional case. A condition of hyperbolicity has been formulated for the two-phase model for a range of parameters specified by the equation of state.

Probably it is possible to generalize a three-dimensional variant of the model [2] to the multi-phase case (in fact, after the manuscript has been prepared, the author received an information from Prof. E. Romensky that a generalization of the prototype model [6] has been conducted in [10]); however, the thermodynamic identity cannot be generalized in the same manner because in the present case the force-energy link is scalar and this fact has been essentially employed in the present report; whereas in the three-dimensional case this link is of essential tensorial nature.

It would be interesting to check out if the generalized specific energy E could be selected as a general dependence upon the specific diffusion velocity v_i. The present selection as the quadratic dependence reflects consistency with the inter-phase behaviour and it has been used for the design of the model, but this dependence is not necessary from the point of view of thermodynamics of the averaged mixture. In that case this dependence could be treated as a specific form of the generalized equation of state.

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19. ABSTRACT

The publication describes a convenient form of one-dimensional equations describing the multi-phase flows associated with the initiation of novel warheads. The model, which has been proposed earlier for the case of two phases, is extended to the case of multi-phase flows. The generalized pressure and energy, which are used in the theory of mixtures, are linked through a thermodynamic potential within the present formulation.